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Small amplitude gasdynamic disturbances in an exploding atmosphere

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The propagation of disturbances through an atmosphere that is, in its undisturbed condition, undergoing a spatially uniform chemical explosion is analysed on the assumption that the disturbances are of small amplitude. When the latter are arbitrarily small, and therefore classifiable as acoustic, the progress of the ambient explosion is undisturbed to first order and a rather complete history of the acoustic waves (including weak shock waves) can be constructed. The generally amplifying effect of the explosion on the disturbances, which has previously been identified at wave heads, is found to occur throughout the disturbed domains.

When the disturbance amplitude becomes comparable to the ratio of the thermal energy of the gas to the combustion–reaction activation energy, the ambient explosion becomes involved in the disturbance to first order. For large activation energies a small disturbance theory can be constructed to account for the disturbance behaviour; at present it is limited to time intervals from initiation that are shorter than the 'no-depletion' homogeneous ignition time.

1. Introduction

Some previous work by the writer (Clarke 1977, 1978) has been aimed at an understanding of the interaction between compression or expansion waves and the homogeneously exploding atmosphere through which they are presumed to propagate. By confining attention to the head of such disturbances it has been possible to draw some useful conclusions in an analytical or near-analytical manner, with the sole assumption that transport effects (mass diffusion, viscosity, heat conduction) are negligible.

If the complete disturbance, from its head to its tail, is presumed to be of limited amplitude one can deploy the techniques of small disturbance theory and thereby analyse the whole disturbed domain provided, once again, that transport effects are negligible.

The following work deals first with arbitrarily small (acoustic) amplitude disturbances, and then goes on to identify a not-so-small disturbance situation in which amplitudes are comparable to an inverse (dimensionless) activation energy for the combustion, or explosion, reaction. Some of the essential features of expansion and compression (including shock) wave behaviour are discussed. The amplifying effect of the explosion is a central feature of all phenomena.

2. Conservation equations

The conservation equations governing the motion of plane, or purely time-dependent, processes in a chemically reacting atmosphere can be written as follows:

$$\rho_t + u\rho_x + \rho u_x = 0, \tag{1}$$

$$\rho u_t + \rho u u_x + p_x = 0, \tag{2}$$

$$c_t + u c_x + \mathscr{R} = 0, \tag{3}$$

$$\{p_t + (u \pm a_f)\, p_x\} \pm \rho a_f \{u_t + (u \pm a_f)\, u_x\} - q\mathscr{R} = 0, \tag{4a, b}$$

where one must take either upper signs, giving (4*a*), or lower signs, giving (4*b*). The quantities p, ρ, u, c and a_f are, respectively, the pressure, density, gas velocity, fuel-species mass fraction and frozen sound speed; the last quantity is given by

$$a_f^2 = \gamma/\rho\beta_f, \quad \rho\beta_f \equiv (\partial\rho/\partial p)_{\tilde{T}, c}, \tag{5}$$

where γ is the ratio of the frozen specific heats and β_f is the frozen isothermal compressibility ($\tilde{T}$ is the absolute temperature). The quantity q is

$$q \equiv \rho(\gamma - 1)\,(\alpha_f \tilde{T})^{-1}\,(\partial h/\partial c)_{p,\,\rho}, \quad \rho\alpha_f \equiv -(\partial\rho/\partial\tilde{T})_{p,\,c}, \tag{6}$$

where h is the enthalpy of the mixture and α_f is the frozen volume expansion coefficient. $\mathscr{R}$ is the rate of progress of a simple nth-order decomposition $nF \rightleftharpoons P$ of n fuel molecules F into the product species P, namely

$$\mathscr{R} = nW\Omega[c^n - (1 - c - c_D)\,\delta]. \tag{7}$$

W is the molecular weight of F, c_D is the (constant) mass fraction of an inert diluent gas and Ω and δ are a chemical frequency and the equilibrium 'constant', respectively.

Equations (4*a*, *b*) make it clear that the characteristics of the equation system lie along

$$dx/dt = u \pm a_f \tag{8a, b}$$

and that wavelets propagating with a local speed a_f relative to the gas velocity u therefore play an important part in transmitting disturbances through the mixture.

The following work will be entirely concerned with the propagation of small-amplitude disturbances (although their nonlinear behaviour is to be emphasized) superimposed upon a background ambient atmosphere undergoing a spatially homogeneous explosion. The special homogeneous-explosion versions of (1)–(4) have zero values for all x derivatives, and are accordingly

$$u = u_0(t) = 0, \quad \rho = \rho_0(t) = \text{constant} = \rho_i, \tag{9a, b}$$

$$p_{0t} - q_0\mathscr{R}_0 = 0, \quad c_{0t} + \mathscr{R}_0 = 0, \tag{9c, d}$$

where $p = p_0(t)$ and $c = c_0(t)$; q_0 and $\mathscr{R}_0$ are the relevant special values of q and $\mathscr{R}$.

Clearly $a_f = a_{f0}(t)$ in this ambient atmosphere, so that in the absence of any perturbations to the ambient state (8*a*, *b*) reduce to

$$dx/dt = \pm a_{f0}(t) \tag{10a}$$

and the related characteristic lines, or frozen wavelets, become

$$x \mp \int_0^t a_{f0}(\hat{t})\, d\hat{t} = \text{constant}. \tag{10b}$$

In order to deal with those nonlinear effects, which arise from the difference between the propagation speeds (8) and (10), it is therefore necessary to take as a new set of independent variables the dimensionless pair (ξ, T) defined as follows:

$$a_{fi}\xi = \mathscr{R}_i g_\xi(\epsilon)\left\{\int_0^t a_{f0}(\hat{t})\,d\hat{t} - x\right\}, \tag{11}$$

$$T = \mathscr{R}_i g_T(\epsilon)\,t, \tag{12}$$

where a_{fi} is the initial value of a_{f0}, namely $a_{f0}(0)$, and $\mathscr{R}_i$ is a typical value of the rate of progress of the chemical reaction. The dimensionless scale factors g_ξ and g_T are functions of a small parameter ϵ that measures the magnitude of the gasdynamic disturbance to the exploding atmosphere, and both are to be found in the course of the analysis. An over-riding requirement for g_ξ and g_T can be quoted in the form

$$g_T/g_\xi = o(1) \quad \text{as} \quad \epsilon \to 0. \tag{13}$$

3. Approximate equations for acoustic-level distributions

The variables p, ρ, u and c are assumed to vary from their ambient values by arbitrarily small amounts; accordingly one can write

$$p(x,t) = p_0(t) + \rho_i a_{fi}^2 g_p(\epsilon)\,p^{(1)}(\xi, T), \tag{14}$$

$$\rho(x,t) = \rho_i\{1 + g_\rho(\epsilon)\,\rho^{(1)}(\xi, T)\}, \tag{15}$$

$$c(x,t) = c_0(t) + g_c(\epsilon)\,c^{(1)}(\xi, T), \tag{16}$$

$$u(x,t) = a_{fi}\, g_u(\epsilon)\,u^{(1)}(\xi, T), \tag{17}$$

where a_{fi} is the value of the frozen sound speed in the spatially homogeneous atmosphere at time zero. The frozen sound speed is also written as

$$a_f(x,t) = a_{f0}(t) + a_{fi}\, g_a(\epsilon)\, a_f^{(1)}(\xi, T). \tag{18}$$

The dimensionless gauge factors $g_\psi(\epsilon)$ $(\psi = p, \rho, c, u, a)$ all depend upon a small parameter ϵ, to be defined more carefully later on, and are all $o(1)$ in the limit as $\epsilon \to 0$. The dimensionless coefficient functions $p^{(1)}$, $\rho^{(1)}$ etc. are therefore only the first approximations to the disturbances imposed upon the ambient exploding atmosphere (the definitions in (14)–(18) would be quite general if $p^{(1)}$ etc. were shown to depend upon the g_ψ factors as well as on ξ and T). A solution is now sought for $p^{(1)}$ etc. in the limit as $\epsilon \to 0$ with ξ and T fixed; $p^{(1)}$ etc. and all of their derivatives with respect to ξ and T are assumed to be $O(1)$.

It readily follows from (1) and (2) that

$$g_p = g_\rho = g_u \tag{19}$$

and these equations integrate to give

$$a_{f0}^2\rho^{(1)} = a_{fi}^2 p^{(1)} = a_{fi} a_{f0} u^{(1)}. \tag{20}$$

It is assumed that $\rho^{(1)}$, $p^{(1)}$ and $u^{(1)}$ all vanish identically somewhere in the field (e.g. for all x greater than some chosen value at $t = 0 = T$).

The quantity Γ_f is defined by

$$a_f \Gamma_f \equiv \left[\frac{\partial}{\partial \rho}(\rho a_f)\right]_{s,c} = a_f + \rho\left(\frac{\partial a_f}{\partial \rho}\right)_{p,c} + \rho a_f^2\left(\frac{\partial a_f}{\partial p}\right)_{\rho,c}, \tag{21}$$

where s is the entropy of the mixture; the second version of (21) follows from the fact that a_f^2 is also equal to $(\partial p/\partial \rho)_{s,c}$. Making use of (19), one can write

$$a_{fi} g_a a_f^{(1)} = \left(\frac{\partial a_f}{\partial \rho}\right)_{p,c|0} g_u \rho_i \rho^{(1)} + \left(\frac{\partial a_f}{\partial p}\right)_{\rho,c|0} g_u \rho_i a_{fi}^2 p^{(1)} + a_{fi} \Delta_0 g_c c^{(1)}, \tag{22}$$

where $$a_{fi} \Delta_0 \equiv (\partial a_f/\partial c)_{p,\rho|0}.$$

It then follows by using (20) and (21) that

$$a_{fi} g_a a_f^{(1)} = g_u(\Gamma_{f0} - 1) a_{fi} u^{(1)} + a_{fi} \Delta_0 g_c c^{(1)}. \tag{23}$$

Γ_{f0} is the value of Γ_f in the ambient, but time-varying, atmosphere.

Now consider (4a) and observe from (9c), (11) and (12) that it can be written in the form

$$\begin{aligned}\{g_\xi a_{f0}(p-p_0)_\xi + g_T a_{fi}(p-p_0)_T - g_\xi(u+a_f)(p-p_0)_\xi\}& \\ + \rho a_f\{g_\xi a_{f0} u_\xi + g_T a_{fi} u_T - g_\xi(u+a_f) u_\xi\} - (a_{fi}/\mathscr{R}_i)\{q\mathscr{R} - q_0\mathscr{R}_0\} &= 0,\end{aligned} \tag{24}$$

since p_0 does not depend upon x. Making use of (14)–(18) and the results contained in the subsequent equations, (24) reduces to

$$\begin{aligned}g_T g_u p_T^{(1)} - g_\xi g_u^2 \Gamma_{f0} u^{(1)} p_\xi^{(1)} - g_\xi g_u g_c \Delta_0 c^{(1)} p_\xi^{(1)}& \\ + a_{f0} a_{fi}^{-1}\{g_T g_u u_T^{(1)} - g_\xi g_u^2 \Gamma_{f0} u^{(1)} u_\xi^{(1)} - g_\xi g_u g_c a_{fi} \Delta_0 c^{(1)} u_\xi^{(1)}\}& \\ - (\rho_i a_{fi}^2 \mathscr{R}_i)^{-1}\{q\mathscr{R} - q_0\mathscr{R}_0\} &= 0.\end{aligned} \tag{25}$$

Only the most significant part of each term of (24) is retained in (25), on the basis of the hypothesis that each of g_u and g_c and hence also g_a is $o(1)$.

At this stage it is appropriate to expand the difference $q\mathscr{R} - q_0\mathscr{R}_0$ as follows:

$$q\mathscr{R} - q_0\mathscr{R}_0 \simeq (q\mathscr{R})_{p0} g_u \rho_i a_{fi}^2 p^{(1)} + (q\mathscr{R})_{\rho 0} g_u \rho_i \rho^{(1)} + (q\mathscr{R})_{c0} g_c c^{(1)} + \ldots, \tag{26}$$

where $(q\mathscr{R})_{p0}$ is written for $(\partial(q\mathscr{R})/\partial p)_{\rho,c}$ evaluated in the time-varying ambient atmosphere, with comparable definitions for $(q\mathscr{R})_{\rho 0}$ and $(q\mathscr{R})_{c0}$. With (20), (26) becomes

$$q\mathscr{R} - q_0\mathscr{R}_0 \simeq g_u \rho_i a_{fi} a_{f0} \mathscr{A}_0 u^{(1)} + (q\mathscr{R})_{c0} g_c c^{(1)}, \tag{27}$$

where $$\mathscr{A}_0 \equiv (q\mathscr{R})_{p0} + a_{f0}^{-2}(q\mathscr{R})_{\rho 0}. \tag{28}$$

The one equation that has not so far been examined in the light of the small-disturbance idea is (3), which, in view of (9d) and the fact that c_0 does not depend upon x, can be written in the form

$$(c-c_0)_t + u(c-c_0)_x + \mathscr{R} - \mathscr{R}_0 = 0. \tag{29}$$

Using (14)–(17), and the relevant results that follow these equations, (29) can be written as

$$g_c g_\xi \mathscr{R}_i a_{f0} a_{fi}^{-1} c_\xi^{(1)} + (\mathscr{R})_{p0} \rho_i a_{fi} a_{f0} g_u u^{(1)} + (\mathscr{R})_{\rho 0} \rho_i a_{fi} a_{f0}^{-1} g_u u^{(1)} + (\mathscr{R})_{c0} g_c c^{(1)} \simeq 0. \tag{30}$$

Once again only the most significant terms are displayed, based on $g_u = o(1)$ and condition (13). Furthermore $(\mathscr{R})_{p0}$ etc. have comparable definitions to $(q\mathscr{R})_{p0}$ etc.

The only way in which the rate of change of c can be involved in a non-trivial way with the propagating disturbance is for the product $g_c\, g_\xi$, which denotes the order of magnitude of the first term in (30), to equal g_u and/or g_c. In the latter case $g_\xi = 1$ and combination of (25) and (27) shows that the chemical-source terms, being then $O(g_u)$, dominate the remaining terms, which are essentially $o(g_u)$ in the circumstances. The presumption that all terms such as $\mathscr{A}_0$ or $\rho_i(\mathscr{R})_{\rho 0}$ are made $O(1)$ on division by $\mathscr{R}_i$ is implicit in the foregoing arguments, as it will be in the arguments that follow. Furthermore $q/\rho_i a_{fi}^2$ is properly assumed to be $O(1)$. It is now evidently necessary for $g_c\, g_\xi$ to equal g_u; in addition the nonlinear gasdynamic behaviour can be preserved only if $g_T\, g_u = g_\xi\, g_u^2$, as is evident from (25). The chemical-source terms in (25) [see (27)] are then of a comparable significance only if $g_\xi\, g_u^2 = g_u$. It follows that a consistent and correct scaling for the present problem has

$$g_T = 1, \quad g_\xi = g_u^{-1}, \quad g_c = g_u^2 \equiv \epsilon^2. \tag{31}$$

The value of $g_u \equiv \epsilon$, say, is fixed by the initial-value data.

The combination of (25), (27), (30) and (31) now gives the following pair of equations for $p^{(1)}$, $u^{(1)}$ and $c^{(1)}$:

$$p_T^{(1)} - \Gamma_{f0}\, u^{(1)} p_\xi^{(1)} + a_{f0}\, a_{fi}^{-1}\{u_T^{(1)} - \Gamma_{f0}\, u^{(1)} u_\xi^{(1)}\} - a_{f0}\, a_{fi}^{-1}(\mathscr{A}_0 \mathscr{R}_i^{-1})\, u^{(1)} = 0, \tag{32}$$

$$c_\xi^{(1)} + \rho_i\, a_{fi}^2 \mathscr{R}_i^{-1}\{(\mathscr{R})_{p0} + a_{f0}^{-2}(\mathscr{R})_{\rho 0}\}\, u^{(1)} = 0. \tag{33}$$

The variations in the fuel mass fraction that are associated with the propagating disturbance, namely $\epsilon^2 c^{(1)}$, can be calculated from (33) once the associated velocity perturbations $\epsilon a_{fi}\, u^{(1)}$ are known. Using (20) and (32), $u^{(1)}$ can be found by solving the nonlinear equation

$$u_T^{(1)} - \Gamma_{f0}\, u^{(1)} u_\xi^{(1)} + \tfrac{1}{2}\{(a_{f0}^{-1}\, a_{f0T}) - (\mathscr{A}_0 \mathscr{R}_i^{-1})\}\, u^{(1)} = 0, \tag{34}$$

subject to suitable initial- or boundary-value data.

4. Solution for $u^{(1)}$

With β defined such that

$$(\partial \xi / \partial T)_\beta = -\Gamma_{f0}\, u^{(1)} \tag{35}$$

(34) integrates to give

$$a_{f0}^{\frac{1}{2}}\, u^{(1)} = F(\beta) \exp\left\{\frac{1}{2}\int_0^t \mathscr{A}_0(\hat{t})\, d\hat{t}\right\}. \tag{36}$$

(N.B. (12) and (31) show that $T\mathscr{R}_i^{-1} = t$.) With $u^{(1)}$ regarded as a function of β and T it is evident that $F(\beta)$ is just the value of $a_{f0}^{\frac{1}{2}}\, u^{(1)}$ when $t = 0$. Writing this quantity as $a_{fi}^{\frac{1}{2}}\, u_i^{(1)}(\beta)$ it follows that (36) gives

$$u^{(1)} = u^{(1)}(\beta, T) = u_i^{(1)}(\beta)\, a_{fi}^{\frac{1}{2}}\, a_{f0}^{-\frac{1}{2}} \exp\left\{\frac{1}{2}\int_0^t \mathscr{A}_0(\hat{t})\, d\hat{t}\right\}. \tag{37}$$

Combination of (35) and (37) leads to the following relation between x, t and β, where β is chosen to have the value $-x$ when $t = 0$:

$$\int_0^t a_{f0}(\hat{t})\, d\hat{t} - x = \beta - \epsilon a_{fi}\, u_i^{(1)}(\beta) \int_0^t \Gamma'_{f0}\, a_{fi}^{\frac{1}{2}}\, a_{f0}'^{-\frac{1}{2}} \exp\left\{\frac{1}{2}\int_0^{t'} \mathscr{A}_0(\hat{t})\, d\hat{t}\right\} dt' \tag{38}$$

[(11) has been used, together with (31)].

From (37), $\partial u^{(1)}/\partial x$ at fixed t is proportional to $(\partial u_i^{(1)}/\partial\beta)\beta_x$, where β_x is written for $\partial\beta/\partial x$ at fixed t. Equation (38), with (37), shows that

$$\beta_x = -\left\{1-\epsilon a_{fi}\int_0^t \Gamma'_{f0}\, u_\beta^{(1)}(\beta, t')\, dt'\right\}^{-1}, \tag{39}$$

so that any compression wave, for which $u_\beta^{(1)} > 0$, must eventually lead to a shock wave after a sufficient lapse of time since β_x must ultimately become unbounded. When $\mathscr{A}_0$ is positive, as it certainly is for the case of a chemically irreversible explosion reaction, for example (Clarke 1978), (37) indicates that $|u_\beta|$ is most likely to increase rapidly from its initial value $|u_{i\beta}|$; the small reduction due to the likely increase in a_{f0} with time is more than offset by the behaviour of the exponential.

Since, at a fixed time,

$$\frac{\partial u}{\partial x} = \epsilon a_{fi}\frac{\partial u^{(1)}}{\partial\beta}\frac{\partial\beta}{\partial x}$$

it follows from (37) and (39) that

$$\frac{\partial u}{\partial x} = \frac{-u_{i\beta}\, a_{fi}^{\frac{1}{2}}\, a_{f0}^{-\frac{1}{2}} \exp\left\{\frac{1}{2}\int_0^t \hat{\mathscr{A}}_0\, d\hat{t}\right\}}{1-u_{i\beta}\displaystyle\int_0^t \Gamma'_{f0}\, a_{fi}^{\frac{1}{2}}\, a'^{-\frac{1}{2}}_{f0} \exp\left\{\frac{1}{2}\int_0^{t'} \hat{\mathscr{A}}_0\, d\hat{t}\right\} dt'}\,. \tag{40}$$

With a few notational changes (40) is identical with the exact result obtained at a wave head whose location is marked by a discontinuity in $\partial u/\partial x$ (Clarke 1977). It is here extended to apply throughout the domain of the disturbance on the understanding that the latter is small (i.e. $u/a_{fi} = O(\epsilon)$) and provided that $\beta_x \neq 0$. The fitting of shock waves into domains for which the inequality is violated will be discussed briefly below. Further limitations on the present results will also be described subsequently.

It must be remarked in passing that the result displayed in equation (42) of the 1977 paper by the writer is unnecessarily complicated by the existence of a term which appears there as

$$(a_{fi}/a_{f0}) \exp\left\{\int_{t_i}^t \Lambda_2(\hat{t})\, d\hat{t}\right\}$$

and which happens to be equal to unity!

5. Illustrative examples

The analysis leading to solutions like (37) and (38), for example, is of a fairly general character, especially in so far as the reaction term $\mathscr{R}$ is concerned. It is now expedient to choose a special form for $\mathscr{R}$ which is a close model of physico-chemical reality and is also such as to make evaluation of terms like

$$\exp\left\{\frac{1}{2}\int_0^t \hat{\mathscr{A}}_0\, d\hat{t}\right\}$$

relatively simple. The model, already used by the writer for a similar purpose (Clarke 1978), makes δ in (7) zero and expresses the frequency Ω as $\mathscr{P}\exp(-\rho E_A/p)$, where $\mathscr{P}$ is a constant pre-exponential factor and E_A is the activation energy of the (now irreversible) burning reaction. Coupled with the assumption that the specific-heat ratio

γ and the 'energy of formation' $(\partial h/\partial c)_{p,\rho}$ are both constant while $\alpha_f \hat{T} = 1$ and $\rho\beta_f = \rho/p$, the combination of (5)–(7) leads to the result that

$$\left(\frac{a_{fi}}{a_{f0}}\right)^{\frac{1}{2}} \exp\left\{\frac{1}{2}\int_0^t \hat{\mathscr{A}}_0\, d\hat{t}\right\} = \left(\frac{p_0}{p_{0i}}\right)^{(2-\gamma)/4\gamma} \exp\left\{\frac{(\gamma-1)}{2\gamma}\rho_i E_A\left(\frac{1}{p_{0i}}-\frac{1}{p_0}\right)\right\}, \tag{41}$$

where p_{0i} is the initial value $p_0(0)$ of $p_0(t)$.

Observe that none of the foregoing results makes any demands about the size of $\rho E_A/p$, although one may certainly demand that it is not negative; we shall find it necessary to comment on the relative sizes of $\rho E_A/p$ and ϵ later on. The geometric shape or extent of the disturbance is strongly influenced by the integral of Γ_{f0} times the expression in (41), as can be seen by consulting (38). With constant γ, Γ_{f0} becomes just $\frac{1}{2}(\gamma+1)$, so that one is then concerned with the value of I, where

$$I \equiv \int_0^t a_{fi}^{\frac{1}{2}} a_{f0}'^{-\frac{1}{2}} \exp\left\{\frac{1}{2}\int_0^{t'} \hat{\mathscr{A}}_0\, d\hat{t}\right\} dt' \tag{42}$$

in the present circumstances. As shown previously (Clarke 1978), it is convenient to calculate I/t_{ign}, where t_{ign} is called the ignition time, which in this case has the value

$$t_{\text{ign}} = \left[\rho_i(\gamma-1)\left(\frac{\partial h}{\partial c}\right)_{p,\rho}\right]^{n-1} \frac{1}{nW\mathscr{P}} \frac{p_{0i}}{\rho_i E_A}\left(\frac{p_{0m}}{p_{0i}}-1\right)^{-n} p_{0i}^{1-n} \exp\left(\rho_i E_A/p_{0i}\right) \tag{43}$$

(p_{0m} is the maximum, final, pressure in the homogeneous explosion).

The information contained in (38) can now be re-presented in the form

$$\left(\int_0^t a_{f0}\, d\hat{t} - x\right) - \beta = -\epsilon a_{fi} t_{\text{ign}}\, \tfrac{1}{2}(\gamma+1)\, u_i^{(1)}(\beta)\, (I/t_{\text{ign}}) \tag{44}$$

and I/t_{ign} is plotted *vs.* t/t_{ign} in figure 1 for various values of $\rho_i E_A/p_{0i}$. In fact it is rather more convenient to plot $(I-t)/t_{\text{ign}}$ and figure 1 depicts this number as well as the explosion pressure and the associated velocity-amplitude factor. The latter is just the ratio $u^{(1)}/u_i^{(1)}$ from (37), which has the specific form given in (41) in the present case. The explosion pressure history has been calculated numerically from (9*c*, *d*) with the 'rate-function' $\mathscr{R}$ as described above.

Figure 1 (*b*) shows that the magnitude of an initial disturbance is increased by the homogeneous explosion, the extent of the amplification depending strongly upon the initial relative activation energy $\rho_i E_A/p_{0i}$. The asymptotic value of the amplification is found by putting $p_0 = p_{0m}$ in (41). On a given wavelet or characteristic β is fixed and its shape on an x, t picture is given by (44). Figure 1 (*c*) shows that I increases more rapidly than t, which is the value of I when the system is chemically inert and there is no change in the ambient state. In a wholly expansive disturbance, for which $u_i(\beta)$ falls monotonically from zero at the wave head to some value $u_i(\beta_e) < 0$ at the tail of the wave, it can be seen from (44) that the characteristics spread out more rapidly than they would otherwise do in an inert atmosphere as a result of this behaviour of I. This extra spreading-out of the simple expansion does not wholly compensate for the amplification of the gas velocity and it can be inferred, from (40) and the results in (44) and figures 1 (*b*) and (*c*), that the ambient explosion processes act to increase the local magnitude of both *u and* $\partial u/\partial x$. The head of the expansion ($\beta = 0$, say) propagates with the time-varying speed a_{f0}, while the tail, at β_e, travels

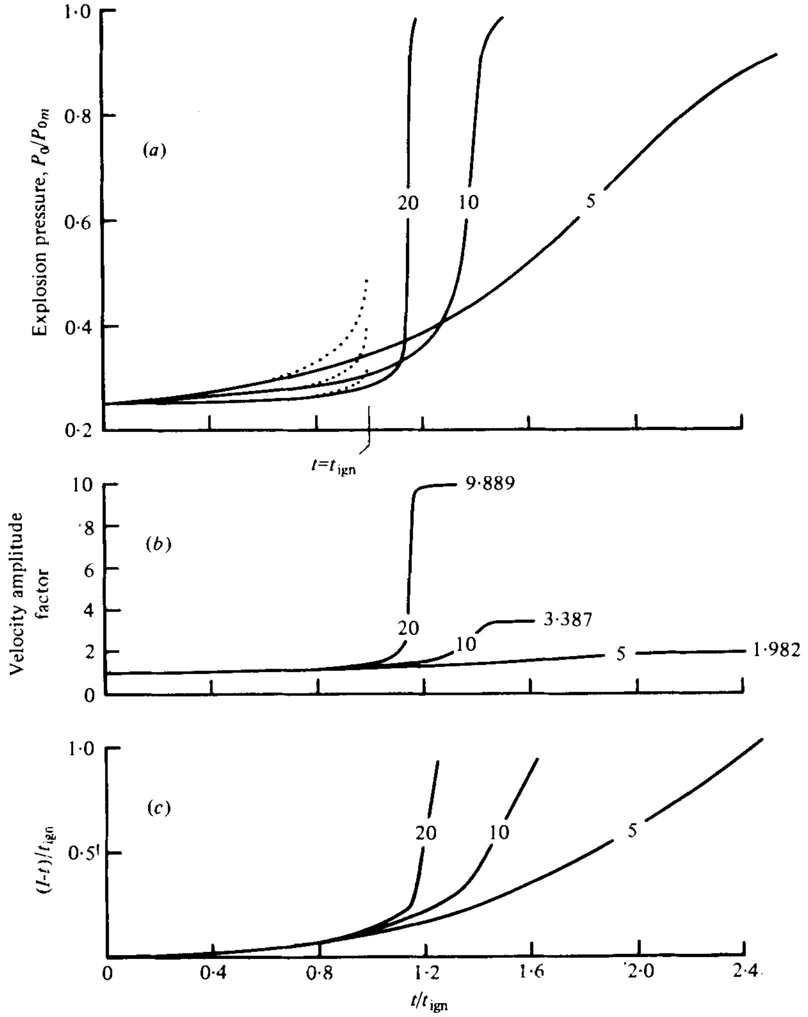

FIGURE 1. (*a*) The pressure *vs.* time in a homogeneous explosion (constant-density process) supported by a first-order chemically irreversible reaction for three values (5, 10 and 20) of the dimensionless activation energy $\rho_i E_A/p_{0i}$. The full lines are derived from numerical integration of (9*c*, *d*) combined with (50) and to that extent illustrate the exact solution; the dotted lines are from the no-depletion approximation (63). The ignition time t_{ign} is defined in (43). (*b*) The velocity amplification factor *vs.* time according to the acoustic theory [see (37)]. (*c*) The integral I [defined in (42)] *vs.* time. I is an important factor in the shape of characteristics [see (44)] and shock waves [see (49), for example] on an x, t picture for acoustic disturbance amplitudes.

at the slower speed $a_{f0}+\epsilon a_{fi}u_i^{(1)}(\beta_e)\,dI/dt$ (remember that $u_i^{(1)} < 0$). Since perturbations to ambient values are essentially limited in scale to $O(\epsilon)$ the tail of the wave must still propagate in the $+x$ direction for the present theory to be valid. It is interesting to speculate on what may happen if ϵ is not limitingly small and dI/dt becomes very large, as it will when $\rho_i E_A/p_{0i}$ is large. It is also interesting to observe that the gas velocity behind (i.e. to the left of) the present isolated expansion must become more negative with time through the agency of the explosion processes; if the expansion is produced by a piston retreating into $x < 0$ then the piston must accelerate; if it does not do so and continues to travel at the velocity $\epsilon a_{fi} u_i^{(1)}(\beta_e)$ there must be a compensatory compression wave generated between the piston face and the expansion. Such matters may be important for explosions taking place within confined spaces whose volume changes with time.

This is perhaps an appropriate place to introduce the question of shock waves. It has already been remarked that a compression will steepen as time proceeds, and that the present solution will fail locally where β_x becomes unbounded (see (39) *et seq.*). The present model allows a more specific interpretation of the latter result, namely that a shock will form on a characteristic β when

$$\epsilon a_{fi} u_{i\beta}^{(1)} \tfrac{1}{2}(\gamma + 1) I = 1.$$

Since $I > t$ for all $t > 0$ this condition must ultimately be met for any positive $u_{i\beta}$ values.

If the local chemical time is long compared with the time of passage of an element of gas through a conventional diffusion-resisted shock front it will be reasonable to treat the latter as a Rankine–Hugoniot discontinuity across which the chemical composition does not vary. Since the time of passage is measured in only a few mean molecular collision intervals, even for weak waves, and chemical times are invariably many such intervals, the assumption is evidently a good one and will be adopted here. In view of the fact that the characteristics in the present problem have the form given in (44), it is possible to take over the shock-fitting formulae derived by Whitham (1974, p. 334, for example) and to locate the discontinuity where $x = x_s$, defined by

$$\int_0^t a_{f0}\, d\hat{t} - x_s = \beta_1 - \epsilon a_{fi} u_i^{(1)}(\beta_1)\, I \tfrac{1}{2}(\gamma + 1) \tag{45}$$

$$= \beta_2 - \epsilon a_{fi} u_i^{(1)}(\beta_2)\, I \tfrac{1}{2}(\gamma + 1), \tag{46}$$

where β_1 and β_2, the characteristics ahead of and behind the shock, are found from

$$[u_i^{(1)}(\beta_1) + u_i^{(1)}(\beta_2)]\,[\beta_2 - \beta_1] = 2\int_{\beta_1}^{\beta_2} u_i^{(1)}(a)\, da. \tag{47}$$

As a simple example consider the initial state

$$u_i^{(1)} = \left\{\begin{matrix} 1 & \text{for} & \beta > 0, \\ 0 & \text{for} & \beta < 0. \end{matrix}\right\} \tag{48}$$

Combination of (45)–(48) then shows that

$$x_s = \int_0^t a_{f0}\, d\hat{t} + \tfrac{1}{4}\epsilon a_{fi}(\gamma + 1)\, I(t). \tag{49}$$

The gas velocity behind the shock at any time is given by (41) times ϵa_{fi} in these circumstances. Figures 1 (*b*) and (*c*) illustrate how the shock wave described by (49) is accelerated and strengthened by the ambient explosive atmosphere.

6. Not-so-small perturbations

There is a tacit assumption in the foregoing work that ϵ is small enough to make the perturbation analysis valid. Some idea of the restrictions implied by the phrase 'small enough' can be understood in the light of the particular results given in the last section, but it is necessary to go back to the development of the difference $q\mathscr{R}-q_0\mathscr{R}_0$ as a Taylor series in (26) *et seq.* to see the real limitation. As explained in the previous section, the chemical frequency factor Ω may well contain a term $\exp(-\rho E_A/p)$, so that differentiation of $\mathscr{R}$ with respect to p or ρ will lead to the appearance of terms proportional to $(\rho E_A/p)^N\mathscr{R}$, where N is the number of differentiations. Evidently a Taylor-series development such as (26) will be valid only if $\rho E_A\epsilon/p$ is very small (indeed $o(1)$ in the limit $\epsilon\to 0$); in other words, when the basic disturbance amplitude ϵ is as large as a typical value of p/ρ (such as p_{0i}/ρ_i) divided by the activation energy E_A, the analysis of § 3 breaks down. When $\rho_i E_A\epsilon/p_{0i}$ is $O(1)$ as $\epsilon\to 0$ the disturbance imposed on the ambient atmosphere is large enough to interfere with the course of the homogeneous explosion to a first-order extent; this happens as a consequence of the extreme sensitivity of the reaction frequency Ω to changes in temperature when the activation energy is large.

Some progress towards a solution of this problem can be made by examining perturbations from the initial, constant, values of the dependent variables in place of the previous method, in § 3, which examined perturbations from the ambient time-varying field [see (14)–(18)]. The arguments used to develop the scalings are of course very similar to those employed in § 3.

A specific form of $\mathscr{R}$ must be selected in this case, namely

$$\mathscr{R} = nW\mathscr{P}\exp\{-\rho p_{0i}/\epsilon\rho_i p\}c^n, \tag{50}$$

where

$$\epsilon \equiv p_{0i}/\rho_i E_A. \tag{51}$$

With the simplifying assumptions that a_f does not depend upon c while $(\partial h/\partial c)_{p,\rho}$ and γ are constant, the analysis proceeds as follows. First write

$$p = p_{0i}+\epsilon\rho_i a_{fi}^2 p^{(1)}, \tag{52}$$

$$\rho = \rho_i+\epsilon\rho_i\rho^{(1)}, \tag{53}$$

$$u = \epsilon a_{fi}u^{(1)}, \tag{54}$$

$$c = c_0(t)+\epsilon^2 c^{(1)}, \tag{55}$$

where the quantities with superscript (1) depend upon ξ and T, which are defined as follows:

$$\epsilon a_{fi}\xi \equiv \hat{\mathscr{R}}_i(a_{fi}t-x), \quad T = \hat{\mathscr{R}}_i t. \tag{56a, b}$$

$\hat{\mathscr{R}}_i$ is defined by

$$\hat{\mathscr{R}}_i \equiv q_i\mathscr{R}_i/\epsilon\rho_i a_{fi}^2 = (q_i/\rho_i a_{fi}^2)\,nW\mathscr{P}e^{-1/\epsilon}\epsilon^{-1}c_{0i}^n \tag{56c}$$

with

$$q_i \equiv \rho_i(\gamma-1)\,(\partial h/\partial c)_{p,\rho}. \tag{56d}$$

Since (9*c*, *d*) show that $q_i c_{0i} = p_{0m}-p_{0i}$ when q_0 = constant = q_i, comparison of (43) and (56*c*) shows that

$$\hat{\mathscr{R}}_i = 1/\gamma t_{\text{ign}}. \tag{57}$$

The foregoing variables, together with (1), (2) and the limit $\epsilon\to 0$ with ξ and T fixed, show that

$$\rho^{(1)} = u^{(1)}(\xi, T), \tag{58}$$

$$p^{(1)} = u^{(1)}(\xi, T)+f(T), \tag{59}$$

where $f(T)$ in (59) is evidently proportional to the perturbation to the initial pressure that arises from the homogeneous explosion [cf. (14) and (20)]. With the aid of (58) and (59), (4*a*) can now be reduced to the following nonlinear equation for $u^{(1)}$:

$$2(\partial u^{(1)}/\partial T)_\beta = \exp\{(\gamma-1)\,u^{(1)}+\gamma f\}-f_T, \tag{60a}$$

$$(\partial\xi/\partial T)_\beta = -\Gamma_{fi}u^{(1)}-\tfrac{1}{2}\gamma f. \tag{60b}$$

Since f must obey the version of (60*a*) that has $u^{(1)}\equiv 0$, (60*a*) can be integrated to give

$$\exp[-(\gamma-1)\,u^{(1)}]-1 = \{\exp[-(\gamma-1)\,u_i^{(1)}(\beta)]-1\}\exp\{\tfrac{1}{2}(\gamma-1)f\}, \tag{61}$$

where $f(0) = 0$ by hypothesis; $u_i^{(1)}(\beta)$ is the initial value of $u^{(1)}$, so that (61) gives $u^{(1)}$ as a function of the parameter β and of f. The latter is a function of T derived from the elementary equation $f_T = \exp(\gamma f)$, namely

$$\gamma f = -\ln(1-\gamma T). \tag{62}$$

From (56*b*) and (57) it can be seen that $f\to\infty$ as $t\to t_{\mathrm{ign}}$; the latter is the estimate of the ignition time based upon the (rather poor) assumption of no reactant depletion ($c_0 \simeq c_{0i}$).

Evidently f grows steadily with increasing T. Combining (59) and (62) with (51) and (52) shows that the homogeneous-explosion pressure is given by

$$p = p_{0i}\{1-(p_{0i}/\rho_i E_A)\ln(1-\gamma T)\} \tag{63}$$

and this result is depicted in figure 1 (*a*); it also serves to illustrate the failure of the zero-depletion approximation as $t\to t_{\mathrm{ign}}$.

The solution for $u^{(1)}$ must be completed by integrating (60*b*) to give the parameter β as a function of ξ and T. To this end (61) and (62) can be rewritten in the form

$$-(\gamma-1)\,u^{(1)} = \ln\{1+(\exp[-(\gamma-1)\,u_i^{(1)}]-1)\,(1-\gamma T)^{-(\gamma-1)/2\gamma}\}, \tag{64}$$

and it is evidently possible to proceed to the required result even if only via numerical quadrature.

Equation (64) reveals two important results rather readily. First, if $u_i^{(1)}(\beta) < 0$ then $u^{(1)}(\beta, T)$ grows more negative as T increases; the associated gasdynamic disturbance is an expansion which is evidently amplified in intensity by its interaction with the explosion; solution (64) breaks down only as $\gamma T \equiv t/t_{\mathrm{ign}}\to 1$. This result is in general accord with the acoustic disturbance theory; only the detailed structure of the expansion will be different. Second, if $u_i^{(1)}(\beta) > 0$, signifying the presence of a compression, solution (64) begins to fail, in the sense that $u^{(1)}\to\infty$ as $T\to T_c$, where

$$(1-\gamma T_c)^{(\gamma-1)/2\gamma} = 1-\exp[-(\gamma-1)\,u_i^{(1)}(\beta)]. \tag{65}$$

This unbounded growth of $u^{(1)}$ can be construed as an indicator of the onset of local explosion, with an accuracy comparable to that involved in the elementary no-depletion model. If $u_i^{(1)}(\beta) = 1, 2,$ or 3 and $\gamma = 1{\cdot}4$, (65) shows that

$$(1-\gamma T_c) \equiv 1-t_c/t_{\mathrm{ign}} \simeq 4{\cdot}2\times 10^{-4},\ 1{\cdot}5\times 10^{-2} \quad\text{or}\quad 8{\cdot}1\times 10^{-2}.$$

The compression is evidently reducing the 'time to ignition' but not, it would appear, in any very dramatic way according to the present theory, whose basic invalidity in the vicinity of t_c or t_{ign} must be emphasized (see figure 1 (*a*), for example).

It is important to observe that the portent of a localized rapid reaction which occurs as a consequence of a propagating compression wave, as roughly modelled in the foregoing analysis, is a function of the velocity (or temperature) disturbance *amplitude* and not of the *rate* at which $u^{(1)}(\beta)$ changes. It is the latter quantity, specifically $u^{(1)}_{\beta}$, that governs the first appearance of a shock wave within a compression. After some elementary but tedious integrations, etc., it can be shown that $(\partial\xi/\partial\beta)_T$ vanishes when

$$\epsilon a_{fi} t_{\text{ign}} u^{(1)}_{i\beta}(\beta) J(u^{(1)}_i(\beta), T) = 1, \tag{66a}$$

where $$J \equiv \gamma(\gamma+1)\exp[-(\gamma-1)u^{(1)}_i]\int_1^{\nu} \frac{w^{-2\gamma/(\gamma-1)}}{1-\{1-\exp[-(\gamma-1)u^{(1)}_i]\}w}\,dw, \tag{66b}$$

$$\nu = (1-\gamma T)^{-(\gamma-1)/2\gamma},$$

and, as in § 4, $\beta = -x$ when $t = 0$. When $u^{(1)}_{i\beta} > 0$, as it will be in a compression, (66*a*) shows that in general a shock wave will form; to be sure it must do so before $\gamma T = 1$, but that is simply a limitation on the present approximate theory and not on the formation of the shock. It is interesting to observe that the time to shock formation does now depend to some extent upon the value of $u^{(1)}_i(\beta)$, in contrast to the acoustic case in § 4 (see (39) especially), but the role of $u^{(1)}_{i\beta}(\beta)$ is still paramount.

The present theory can really only hint at the manner in which contiguous locations of explosive reactions and shock waves will evolve and interact. However, further developments along the present lines hold out substantial hope for progress in the understanding of these complex processes.

7. Conclusions

When the disturbance amplitude is very small it is possible to construct a complete first approximation to the behaviour of simple waves which propagate at the local frozen sound speed relative to a gas whose ambient state is changing with time. This can be done for all times from the initiation of the explosion, through its intense-reaction (explosive) phase and on to completion of the explosion. The growth of the initial, imposed, spatially non-uniform disturbance follows a simple rule in such a case, as witnessed by (37). The latter result is very general in respects other than that of the acoustic level of the disturbances, since it can account for ambient reactions that are either irreversibly explosive or initially in equilibrium. Principal interest is in the explosive situation, and a few sample calculations illustrate how the ultimate extent of the amplification is strongly dependent on the activation energy, and therefore the temperature sensitivity, of the burning reaction. The two specific examples of an initial expansion and an initial weak-shock compression of the explosive gas show how the presence of solid surfaces may alter the development of the wave in unexpected ways, although these are not worked out here.

If the disturbance amplitude is as large as the inverse of the dimensionless activation energy the acoustic theory must be modified. The disturbance now exerts a first-order influence on the progress of the explosion, via the temperature-sensitive reaction frequency, and a nonlinearity from the chemical processes is fed into the disturbance equations, which already contain the usual convective nonlinearities of a longitudinal wave motion. When attention is confined to times for which reactant depletion is negligible the resulting equations can still be solved analytically. The solutions exhibit the quantitative effects of amplitude, which affect the onset of rapid reaction, and of rates of change of amplitude, which can affect shock formation, provided the time does not approach the (rather artificial) no-depletion ignition time too closely.

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